The spectral computation of birth and death chains

Guan-Yu Chen

Dept. of Applied Math, NCTU

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1. Mixing time for Markov chains
2. Separation mixing of birth and death chains
3. Computing the spectral gap
4. Computing the whole spectrum

Fundamental setting

- $\mathcal{X}$: a finite set.
- K: a matrix indexed by $\mathcal{X}$ satisfying

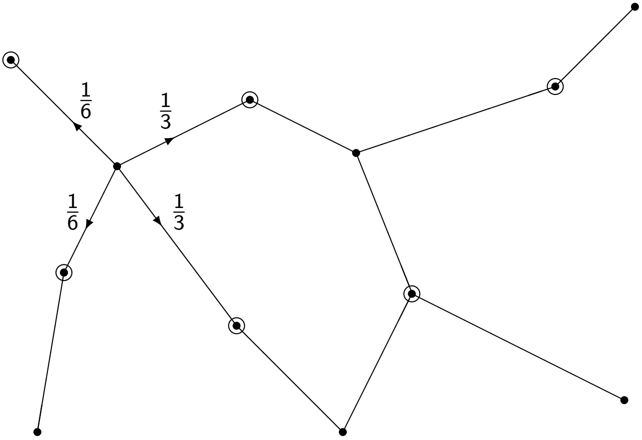
$$K(x,y) \geq 0, \quad \sum_y K(x,y) = 1.$$

- X_m: a (discrete time) Markov chain on $\mathcal{X}$ with transition matrix K. That is,

$$\mathbb{P}(X_{m+1} = y | X_m = x, X_{m-1} = i_{m-1}, ..., X_0 = i_0) = K(x,y).$$

- K is irreducible if, for any $x, y \in \mathcal{X}$, there is $m > 0$ such that $K^m(x,y) > 0$.
- If K is irreducible, then there is a unique probability π on $\mathcal{X}$ satisfying $\pi K = \pi$. π is called the stationary distribution of K.

Random walks on graphs



Converging to the stationarity

Theorem

Let K be irreducible with stationary distribution π. If K is aperiodic, i.e. there is $m > 0$ such that $K^m(x,y) > 0$ for all $x, y \in \mathcal{X}$, then

$$\lim_{m\to\infty} \mathbb{P}(X_m = y | X_0 = x) = \lim_{m\to\infty} K^m(x,y) = \pi(y), \quad \forall x, y \in \mathcal{X}.$$

Measuring the convergence

Let μ be the distribution of X_0.

- Total variation:

$$d_{\text{TV}}(\mu, m) = \|\mu K^m - \pi\|_{\text{TV}} := \max_{A \subset \mathcal{X}} |\mu K^m(A) - \pi(A)|.$$

- Separation:

$$d_{\text{sep}}(\mu, m) = \text{sep}_\pi(\mu K^m) := \max_{y \in \mathcal{X}} \{1 - \mu K^m(y)/\pi(y)\}.$$

- Mixing time: Let d be any above distance. The mixing time in d is defined by

$$T_d(\mu, \epsilon) = \min\{m \geq 0 | d(\mu, m) \leq \epsilon\}, \quad \forall \epsilon > 0.$$

Birth and death chains

Let $n \in \mathbb{N}$.

- $\mathcal{X} = \{0, 1, ..., n\}$.
- Birth rate p_i, death rate q_i and holding rate r_i satisfying

$$p_i + q_i + r_i = 1, \quad p_n = q_0 = 0.$$

- A birth and death chain is a Markov chain on $\mathcal{X}$ with transition matrix K given by

$$K(i, i+1) = p_i, \quad K(i, i-1) = q_i, \quad K(i, i) = r_i.$$

- K is irreducible if $p_i q_{i+1} > 0$ for $0 \le i < n$.
- If K is irreducible, then K is aperiodic if and only if $r_i > 0$ for some i.
- If K is irreducible with stationary distribution π, then

$$\pi(i) = c \frac{p_0 p_1 \cdots p_{i-1}}{q_1 q_2 \cdots q_i},$$

where c is a normalizing constant.

Separation distance

Theorem (Diaconis & Saloff-Coste(2006))

Let K be the transition matrix of an irreducible birth and death chain on $\{0,1,...,n\}$. Let $\lambda_1,...,\lambda_n$ be nonzero eigenvalues of $I-K$. Suppose $p_i+q_{i+1}\le 1$ for $0\le i<n$. Then,

$$d_{\text{sep}}(\delta_0,m)=d_{\text{sep}}(\delta_n,m)=\sum_{i=1}^{n}\prod_{j\neq i}\frac{\lambda_j}{\lambda_j-\lambda_i}(1-\lambda_i)^m,$$

where δ_i is the Dirac measure concentrated on i.

Separation distance

Refer to the setting in the above Theorem.

(1) Let T be a random variable satisfying

$$\mathbb{P}(T > m) = d_{\text{sep}}(\delta_0, m).$$

Then,

$$\mathbb{E}T = \sum_{i=1}^{n} \frac{1}{\lambda_i}, \quad \text{Var}(T) = \sum_{i=1}^{n} \frac{1-\lambda_i}{\lambda_i^2}.$$

(2) If $\lambda_i < 1$ for $1 \le i \le n$, then T is the sum of independent geometric random variables with success probabilities $\lambda_1, \ldots, \lambda_n$.

Separation mixing time

Recall the one-sided Chebyshev inequality. Let $\mathrm{SD}(Y)$ be the standard deviation of a random variable Y. For $a > 0$,

$$\mathbb{P}(Y > \mathbb{E}Y + a\mathrm{SD}(Y)) \le \frac{1}{1+a^2}, \quad \mathbb{P}(Y < \mathbb{E}Y - a\mathrm{SD}(Y)) \le \frac{1}{1+a^2}.$$

This implies, for $\epsilon \in (0,1)$,

$$\lfloor \mathbb{E}T - (1/\epsilon - 1)^{-1/2}\mathrm{SD}(T) \rfloor \le T_{\text{sep}}(\delta_0, \epsilon) \le \lceil \mathbb{E}T + (1/\epsilon - 1)^{1/2}\mathrm{SD}(T) \rceil,$$

where $\lfloor t \rfloor = \max\{z \in \mathbb{Z} | z \le t\}$ and $\lceil t \rceil = \min\{z \in \mathbb{Z} | z \ge t\}$.

Ehrenfest chains

- A lazy Ehrenfest chain on $\{0, 1, ..., n\}$ is a birth and death chain with

$$p_i = 1/2 - i/(2n), \quad q_i = i/(2n), \quad r_i = 1/2.$$

- The stationary distribution π satisfies $\pi(i) = \binom{n}{i} 2^{-n}$.
- The transition matrix of the Ehrenfest chain has eigenvalues $\beta_i = 1 - i/n$ for $0 \le i \le n$ and eigenvectors

$$\psi_i(j) = \binom{n}{i}^{-1/2} \sum_{k=0}^{i} (-1)^k \binom{j}{k} \binom{n-j}{i-k},$$

where ψ_i is related to Krawtchouk polynomials. (Difference relation)

- Clearly, $\mathbb{E}T = n \log n + O(1)$, $\mathrm{SD}(T) \asymp n$ and

$$T_{\text{sep}}(\delta_0, \epsilon) = n \log n + O(n), \quad \forall \epsilon \in (0, 1).$$

Qualitative behavior

Theorem

Let K be the transition matrix of an irreducible birth and death chain on $\{0, 1, ..., n\}$ with rates p_i, q_i, r_i. Let β be an eigenvalue of K with associated eigenvector ψ. Then, for $0 \leq i \leq n$,

$$\beta\psi(i) = p_i\psi(i+1) + q_i\psi(i-1) + r_i\psi(i), \tag{1}$$

where $p_n = q_0 = 0$. Furthermore, if β is the second largest eigenvalue of K and $\psi(0) < 0$, then

$$\psi(i) < \psi(i+1), \quad \forall 0 \leq i < n.$$

Remark

The monotonicity of ψ due to the work of Miclo in 2009.

Qualitative behavior

- If ψ is an eigenvector associated with a non-zero eigenvalue of $I-K$, then $\pi(\psi)=0$.
- Subtracting $\psi(i)$ from both sides of (1) gives

$$\psi(i+1)=\psi(i)+\frac{[\psi(i)-\psi(i-1)]q_i-\lambda\psi(i)}{p_i},$$

  where $\lambda=1-\beta$.
- If β is the second largest eigenvalue of K, then λ is called the spectral gap of K. Furthermore,

$$\lambda=\inf\left\{\frac{\mathcal{E}(f,f)}{\mathrm{Var}_\pi(f)}\middle| f\text{ is non-constant}\right\},$$

  where $\mathcal{E}(f,g):=\langle f,(I-K)g\rangle_\pi$ and $\mathrm{Var}_\pi(f)=\pi(f^2)-(\pi(f))^2$.

Characterizing the spectral gap

Theorem (Chen & Saloff-Coste(2012))

Let λ be the spectral gap of K. For $a > 0$, set $\phi_a(0) = -1$ and

$$\phi_a(i+1) = \phi_a(i) + \frac{\{[\phi_a(i) - \phi_a(i-1)]q_i - a\phi_a(i)\}^+}{p_i},$$

where $t^+ = \max\{t, 0\}$. Set $L(a) = \mathcal{E}(\phi_a, \phi_a)/\mathrm{Var}_\pi(\phi_a)$. Then,

$$L(a) = a \quad \Leftrightarrow \quad \pi(\phi_a) = 0 \quad \Leftrightarrow \quad a = \lambda.$$

Furthermore,

$$\pi(\phi_a) \begin{cases} > 0 & \text{for } a > \lambda, \\ < 0 & \text{for } 0 < a < \lambda. \end{cases}$$

Algorithm 1

Theorem (Chen & Saloff-Coste (2012))

Let L, λ be as in the previous theorem. Fix $a > 0$ and set $\lambda_0 = a$ and $\lambda_{k+1} = L(\lambda_k)$. For $n \geq 2$:

(1) If $a = \lambda$, then $\lambda_k = \lambda$ for all k.

(2) If $a \neq \lambda$, then $\lambda_k > \lambda_{k+1} > \lambda$.

(3) There is $\sigma \in (0, 1)$ such that

$$0 \leq \lambda_k - \lambda \leq \sigma^{k-1}\lambda_1, \quad \forall k \geq 1.$$

Remark

For $n = 1$, $\mathcal{E}(f, f) = \lambda \mathrm{Var}_\pi(f)$ for any f.

Algorithm 2

- Set $L_0 = 0$ and $U_0 = 2$.
- For $k = 0, 1, ...,$ define $\lambda_k = (L_k + U_k)/2$ and

$$\begin{cases} L_{k+1} = L_k, U_{k+1} = \lambda_k & \text{if } \pi(\phi_{\lambda_k}) > 0 \\ L_{k+1} = \lambda_k, U_{k+1} = U_k & \text{if } \pi(\phi_{\lambda_k}) < 0, \\ L_{k+1} = U_{k+1} = \lambda_k & \text{if } \pi(\phi_{\lambda_k}) = 0. \end{cases}$$

Theorem

Referring to the above setting, one has

$$0 \leq \max\{U_k - \lambda, \lambda - L_k\} \leq 2^{1-k}, \quad \forall k \geq 0.$$

Qualitative behavior

Theorem (L. Miclo (2008))

Let K be the transition matrix of a birth and death chain on $\{0, 1, ..., n\}$. For $1 \le i \le n$, let λ_i be the i-th smallest non-zero eigenvalue of $I - K$ and ζ_i be an eigenvalue associated with λ_i satisfying $\zeta_i(1) < 0$. Then, there are

$$0 = a_1 < b_1 \le a_2 < b_2 \le \cdots \le a_i < b_i = n$$

satisfying $a_{j+1} - b_j \in \{0, 1\}$ such that $\zeta_i(b_j) = \zeta_i(a_{j+1})$ and

$$\zeta_i \text{ is strictly } \begin{cases} \text{increasing on } [a_j, b_j] & \text{if } j \text{ is odd,} \\ \text{decreasing on } [a_j, b_j] & \text{if } j \text{ is even.} \end{cases}$$

Vectors of Type i

Definition

A function $f : \{0, 1, ..., n\} \to \mathbb{R}$ is called "Type i" if there are

$$0 = a_1 < b_1 \leq a_2 < b_2 \leq \cdots \leq a_i < b_i \leq n$$

satisfying $a_{j+1} - b_j \in \{0, 1\}$ such that $f(b_j) = f(a_{j+1})$ and

(1) f is strictly monotonic on $[a_j, b_j]$ for all $1 \leq j \leq i$.

(2) $[f(a_j) - f(a_j + 1)][f(a_{j+1}) - f(a_{j+1} + 1)] < 0$.

(3) $f(k) = f(b_i)$ for $b_i \leq k \leq n$.

The points a_j, b_j are called "peak-valley points" of f.

Vectors of Type i

- For $a > 0$, let $\phi_a(0) = -1$ and set

$$\phi_a(i+1) = \phi_a(i) + \frac{[\phi_a(i) - \phi_a(i-1)]q_i - a\phi_a(i)}{p_i}.$$

- Suppose ϕ_a is of type i with peak-valley points $a_1, b_1, ..., a_i, b_i$. For $1 \le j < i$, define

$$\phi_a^{(j)}(k) = \begin{cases} \phi_a(k) & \forall 0 \le k \le b_j, \\ \phi_a(b_j) & \forall b_j < k \le n. \end{cases}$$

  For $i \le j \le n$, set $\phi_a^{(j)} = \phi_a$.

- For $a > 0$, set

$$\mathcal{L}(a) = \frac{\mathcal{E}(\phi_a, \phi_a)}{\text{Var}_\pi(\phi_a)}, \quad \mathcal{L}^{(j)}(a) = \frac{\mathcal{E}(\phi_a^{(j)}, \phi_a^{(j)})}{\text{Var}_\pi(\phi_a^{(j)})}$$

Local convergence

Theorem (Chen & Saloff-Coste (2012))

Let $\lambda_1 < \cdots < \lambda_n$ be the non-zero eigenvalues of $I - K$. Then, there is $\epsilon > 0$ such that, for $1 \le i \le n$ and $|a - \lambda_i| < \epsilon$,

(1) $\phi_a = \phi_a^{(i)}$,

(2) Set $a_0 = a$ and $a_{k+1} = \mathcal{L}(a_k)$. Then, $(a_k)_{k=1}^{\infty}$ is monotonic and converges to λ_i.

Characterizing the spectrum

Theorem (Chen & Saloff-Coste (2012))

Let $\lambda_1 < \cdots < \lambda_n$ be non-zero eigenvalues of $I - K$ and ϕ_a be the vector defined as before. Then, there are constants $\alpha_i \in (\lambda_i, \lambda_{i+1})$ with $1 \le i \le n-1$ such that

(1) ϕ_a is of type i for $a \in (\alpha_{i-1}, \alpha_i]$, where $a_0 := 0$ and $a_n := \infty$.

(2) $\pi(\phi_a) > 0$ for $a \in (\lambda_{2i-1}, \lambda_{2i})$, where $\lambda_0 := 0$ and $\lambda_{n+1} := \infty$.

(3) $\pi(\phi_a) < 0$ for $a \in (\lambda_{2i}, \lambda_{2i+1})$.

Algorithm computing the ith smallest eigenvalue

- Set $L_0 = 0$ and $U_0 = 2$.
- For $k = 0, 1, \ldots$, let $\lambda_k = (L_k + U_k)/2$ and j be the type of ϕ_{λ_k}. Set

$$\begin{cases} L_{k+1} = L_k, U_{k+1} = \lambda_k & \text{if } j > i \text{ or if } j = i,\ (-1)^{i+1}\pi(\phi_{\lambda_k}) > 0, \\ L_{k+1} = \lambda_k, U_{k+1} = U_k & \text{if } j < i \text{ or if } j = i,\ (-1)^{i+1}\pi(\phi_{\lambda_k}) < 0, \\ L_{k+1} = U_{k+1} = \lambda_k & \text{if } j = i,\ \pi(\phi_{\lambda_k}) = 0. \end{cases}$$

Theorem

Let λ_i be the ith smallest non-zero eigenvalue of $I - K$. Then,

$$0 \le \max\{U_k - \lambda_i, \lambda_i - L_k\} \le 2^{1-k}, \quad \forall k \ge 0.$$

Reference

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Thank you!